

**Anomalous Signature of Superfluid Density in the Single Particle Excitation Spectrum of High-Temperature Superconductors**

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We report [1] that the doping and temperature dependence of photoemission spectra near the Brillouin zone boundary of high-temperature superconductors exhibit unexpected sensitivity to the superfluid density. The photoemission peak intensity as a function of doping scales with the superfluid density, the condensation energy and the critical current density. As a function of temperature, the peak shows an abrupt behavior near  $T_C$ , where phase coherence sets in, rather than near  $T^*$  where the gap opens. This anomalous manifestation of superfluidity in the single-particle spectroscopy raises important questions relating to the mechanism of high-temperature superconductivity.

[1]D. L. Feng et al., submitted to "Science", and the references therein.

**Physics of a Mott Insulator: an ARPES Study of Ca<sub>2</sub>CuO<sub>2</sub>Cl<sub>2</sub>**

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ARPES data on Ca<sub>2</sub>CuO<sub>2</sub>Cl<sub>2</sub> has shown a rapid loss in spectral weight as one crosses the antiferromagnetic zone boundary. Moreover, a d-wave-like dispersion was found along this boundary. However, with improved momentum resolution we demonstrate that the dispersion near ( $\pi/2, \pi/2$ ) does not contain a cusp as would be expected from a simple d-wave theory. The rounded node region and the total dispersion of approximately 350meV is also shown to be independent of photon energy despite the fact that the relative spectral weight along the antiferromagnetic zone boundary varies strongly as a function of photon energy.

Observation of Superconducting Gap and in-Gap Bound State of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  Surface

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High-resolution angle-resolved photoemission spectroscopy (ARPES) measurements have been performed on untwinned  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  (Y123) single crystals. By recognizing the narrow intense peak observed at both X and Y point as an in-gap surface bound state, we have for the first time identified a superconducting (SC) peak with a peak-dip-hump structure near  $(\pi, 0)$ . The striking resemblance of this superconducting peak between Y123 and Bi2212 suggests its universality in cuprates superconductors with high- $T_c$ . In addition, strong anisotropy in the electronic structure has been found between a and b direction: the intensity of the SC peak is higher at X point than at Y point while the size of the SC gap is smaller at X point than at Y point. This is consistent with the a-b anisotropy found in the microwave and optical measurements of superfluidity as well as recent neutron scattering results on Y123.

**A New High-Resolution Toroidal Energy- and Angle-Resolved Electron Spectrometer**

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The Toroidal Energy- and Angle-Resolved Electron Spectrometer (TEARES) is a state-of-the-art high-resolution electron detector that is being designed, built and developed at Daresbury Laboratory. The project aims (1) to enhance the range of electron detector systems available at the Synchrotron Radiation Source at Daresbury, (2) to provide a toroidal electron analyser system with simultaneous readout of energy and angle, and (3) to start the development of a fast 2D readout system for electron detector systems that is capable of high dynamic range and matched to the toroidal analyser system. Experiments that would benefit from such a system include photoelectron diffraction from solid surfaces, magnetic dichroism from solid surfaces, 'spin-polarised' studies of surfaces, atomic and molecular physics experiments, and photoelectron spectroscopy where the cross-section is low.

A toroidal energy analyser allows both the energy and angle of ejection of an electron to be measured simultaneously. In the TEARES system, electrons that are ejected in a plane perpendicular to the main axis of the spectrometer will be transported and focussed by cylindrical slit lenses onto the entrance of a toroidal electrostatic analyser. The analyser is comprised on an inner and an outer toroidal sector. Electrons are deflected by the electric field between the two toroids in such a way that only those electrons having energies near the pass energy of the analyser will arrive at the exit cone of the analyser. The toroidal analyser disperses the electrons according to their energy in the radial dimension whilst preserving their angular direction in the angular dimension. The conical exit lenses transport, demagnify, and focus the electrons from the exit of the analyser onto the detector.

The TEARES comprises a double focussing cylindrical slit entrance lens, a toroidal sector deflector, and a conical slit exit lens. The working distance of the system is defined by a 40 mm radius. The spherical radius of the toroidal analyser is 125 mm, the cylindrical radius is 119 mm, and the sector angle is 142 degrees. The latter two dimensions have been chosen to insure optimum focussing properties. The resolution of a toroidal analyser is determined by the spherical radius, pupil, and entrance slit height. A resolution of 4 meV should be possible using 1 mm high entrance slits together with a pass energy of 0.5 eV. The TEARES system is designed to operate over the kinetic energy range of  $0.5 \leq KE \leq 1000$  eV. The active area of the detector has a diameter of 40 mm.

At the present time most commercial detectors are capable of achieving countrates up to 1MHz ( $1 \times 10^6$ ) in imaging

The gas phase  $L_{2,3}VV$  Auger electron spectra of chlorine

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The Auger electron spectra (AES) following the chlorine  $2p$  ionization in the gas phase alkali-chlorides as well as in the HCl and DCl molecules were studied theoretically and experimentally.[1] Non-relativistic *ab initio* calculations based on quantum chemical methods and the one-center approximation were used to compute the  $L_{2,3}VV$  AES. The vibrational band structure in the AES was simulated by full life time vibrational interference (LVI) theory and a more approximate moment method. Calculations were compared with the corresponding experimental electron or photon impact excited spectra. Overall features and changes in the series of the experimental AES are correctly predicted by the theory. For the most intense transitions in these spectra a qualitative explanation of the energies is given on the basis of a model that includes electrostatic interactions, Pauli repulsion and polarization. This explains that the substantial changes of the spectra with X are due to a  $R^{-3}$  dependence of the electrostatic interaction on the X-Cl bond length. Comparison of the two theoretical methods shows that the LVI vibrational band breadths are well reproduced by the moment method in the AES of HCl, DCl, and LiCl, whereas the moment breadths are underestimated in the AES of NaCl and KCl. The LVI band breadths for HCl, DCl and KCl are in good agreement with experimental data. In contrast, the experimental spectra for LiCl and NaCl show almost two times broader vibrational bands than predicted by the LVI theory. This contradiction indicates that the LiCl and NaCl vapors are contaminated by the dimer form of these substances. A large contribution of  $Li_2Cl_2$  (74 %) and  $Na_2Cl_2$  (29 %) was measured in the LiCl and NaCl vapors by time-of-flight mass spectroscopy. The Auger peaks in the spectra of the dimers lie very close to the monomer peaks, and thus makes it very difficult to distinguish dimer and monomer contributions.

[1] Mika Kivilompolo, Antti Kivimäki, Helena Aksela, Marko Huttula, Seppo Aksela, and Reinhold F. Fink, accepted for publication Journal of Chemical Physics

Spin asymmetry in (e, 2e) process on atoms by longitudinally polarized electrons

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We present in this communication the theoretical demonstration of the spin asymmetry in the triple differential K-shell ionization cross-reaction (TDCS) of atoms by longitudinally polarized relativistic electrons. The formalism for the spin asymmetry calculation has been developed in one photon exchange approximation. We have used Dirac plane waves, Darwin wave function and non-relativistic Coulomb wave function multiplied by the Darwin matrix to represent incident and scattered electrons, bound electron and ejected electron, respectively. We will present the results of our calculation of longitudinal spin asymmetry in TDCS as a function of ejected electron angle (with the incident beam direction) by 300 keV incident electron on Cu, Ag and Au targets in coplanar asymmetric geometry. The longitudinal spin asymmetry for Cu target at different scattering electron angles is shown in the fig 1. The calculated longitudinal spin asymmetry is large as compared to the transverse spin asymmetry [1] for the same set of kinematical parameters. The interference between the longitudinal and transverse interaction terms in TDCS of relativistic (e, 2e) collision on atoms is known to explain the observed shift in the binary peak away from the momentum transfer direction as well as formation of the recoil peak [2,3]. We will discuss here the role of the longitudinal, transverse and interference terms in the calculation of longitudinal spin asymmetry. We will also comment upon the difference in the calculated transverse and longitudinal spin asymmetry in the (e, 2e) process on atoms.

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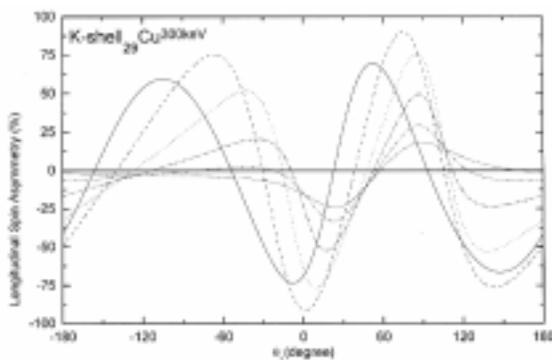


Fig. 1 Longitudinal spin asymmetry of triple differential K-shell ionization cross section of copper as a function of the scattering angle  $\theta_2$  of the ejected electron (incident electron energy  $E_0 = 300$  keV, ejected electron energy  $E_2 = 71$  keV) for  $\theta_1 = -5^\circ$  (—),  $\theta_1 = -10^\circ$  (---),  $\theta_1 = -15^\circ$  (· · · · ·),  $\theta_1 = -20^\circ$  (- - - -),  $\theta_1 = -25^\circ$  (— · — · —), and  $\theta_1 = -30^\circ$  (— · — · —).

**Title in Upper and Lower Case with Any Credits Denoted with an \* Combined Experimental and Theoretical Determination of the 3C-SiC(100) c(4x2) Surface Electronic Band Structure**

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The 3C-SiC(100) surface exhibits several reconstructions ranging from Si-rich to C-rich surfaces. Most of the research has been so far devoted to the geometry of these surfaces, while investigations about surface electronic properties remain limited to very few. The Si-terminated 3C-SiC(100) surface is of special interest since its organization is primarily driven by stress [1,2]. Unlike covalent semiconductor such as Si or Ge (100) surfaces, the room temperature Si-terminated 3C-SiC(100) reconstruction displays a c(4x2) pattern resulting from alternating up- and down-dimers (AUDD) rows as evidenced by scanning tunneling microscopy [1] and by total energy ab-initio calculations [2]. Another model, the missing asymmetric dimer row model (MRAD) was also proposed by pseudopotential calculations [3]. In this paper we investigate the electronic properties of the 3C-SiC(100) c(4x2) surface reconstruction by combined angle resolved ultraviolet photoemission spectroscopy (ARUPS) and electronic structure calculations. Using ARUPS, we have measured electronic bulk and surface states and discuss the dispersion of 4 surface states along the two high symmetry directions of the 2D Brillouin zone. The experimental and theoretical band structures are found to be in very good qualitative and quantitative agreement. The results, which are inconsistent with the MRAD model, strongly support the AUDD picture of the c(4x2) surface [1,2], in excellent agreement with recent core level photoemission spectroscopy measurements [4]. Interestingly, we find a dangling-bond overlap perpendicularly to the dimer row between up- and down dimers belonging to two adjacent rows.

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**Three-dimensional Atomic Imaging of As/Si(111) Using Self-Normalizing Photoelectron Holography**

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Photoelectron holography is a powerful technique that provides species-specific real-space images of surface atomic arrangements. To do this it is necessary to obtain a large set of photoelectron spectra taken over many angles and over a wide range of photon energies. Typically, thousands of spectra are needed. A direct application of the technique uses the intensities of spectral lines. Normalization of these intensities can be a problem because over the course of an experiment it may be necessary to change analyser or monochromator modes to cover the needed

energy range and several synchrotron beam fills may occur during the measurement time. Some way of "splicing" data

sets taken under different conditions must then be used. As an alternative, self-normalizing methods may be employed.

In the present work, two such methods, one based on branching ratios and the other on derivatives, are applied to the As/Si(111) system. The resulting images agree with other experimental and theoretical results, and their quality is such that second-nearest neighbors are resolved. Issues concerning the handling of surface refraction, proper angle and energy windows, and the scattering phase shift are discussed.

**The electronic screening effect in impact-parameter calculations**

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In this work we focus on the electronic screening effect of the projectile on the amplitude of a target atomic transition in the framework of the semiclassical approximation (SCA).

The aim is to elaborate a general tool for accounting projectile electronic screening effect in impact parameter calculations, even when the target or projectile wave functions are numerical. Our calculation is based on Ref. [1]. The method is applicable when the projectile electronic wavefunctions are approximated by Slater-type orbitals [2]. Then the screening potential has the following form:

$$V_s(R-r) = \frac{N}{|R-r|} - \sum_{k=0}^F c_k |R-r|^{n_k-1} e^{-a_k |R-r|},$$

where  $N$  is the number of projectile electrons,  $R$  is the internuclear distance,  $r$  is the projectile electron and nucleus distance,  $F$  is an integer,  $c_k$ ,  $n_k$  are real and  $a_k$  is a positive number. For numerical projectile wave functions we use a nonlinear least-squares fitting technique to estimate the parameters [3].

Following Ref. [1] we utilized the multipole expansion [1]:

$$\frac{e^{-a|R-r|}}{|R-r|} = \sum_{L=0}^{\infty} \frac{2L+1}{\sqrt{Rr}} I_{L+1/2}(ar_{<}) K_{L+1/2}(ar_{>}) P_L(\hat{R} \cdot \hat{r})$$

where  $I_{L+1/2}$  and  $K_{L+1/2}$  are the modified Bessel functions of fractional order, and the identity:

$$x^n e^{-ax} = \frac{d^{n+1}}{d(-a)^{n+1}} \frac{e^{-ax}}{x}.$$

We have elaborated closed expressions, recursive relations and integral representation routines for the  $n$ th order derivation of the modified spherical Bessel function of first and second kind and respectively for their products. Total cross sections are calculated and compared with experimental data and reference theoretical results.

References

**Study of the transfer-loss process in collisions of Li-like ions with light targets at low energies**

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The method of zero-degree projectile Auger spectroscopy was applied earlier to measure the state selective K-shell excitation of the Li-like  $F^{6+}$  and  $O^{5+}$  ions incident with 3 - 10 a.u. velocity on He and  $H_2$  targets [1].

One of the studied process is:



For the projectile final state there exists three alternatives which can be marked with the spectroscopic notations:  $^4P$ ,  $^2P_{-}$  [ $(^3P)^2P$ ],  $^2P_{+}$  [ $(^1P)^2P$ ].

One of the possible mechanism resulting these final states is the so called transfer-loss process (TL): the ionization of a 1s electron of the projectile and the a transfer of a target 1s electron to the projectile 2p shell.

TL is the dominant process for producing the 1s2s2p projectile configuration at low (3 - 10 MeV) impact energies.

We calculate the transfer-loss probability using the independent particle model (IPM) by taking the product of the transfer (capture) and loss (ionization)

probabilities.

$$P_{\{TL\}} = P_{\{T\}} P_{\{L\}}.$$

The cross section for a specific m is:

$$\sigma_{\{TL\}}^{1s2s2p_m} = 2\pi \int_0^\infty db \, b \, P_{\{TL\}}^{1s2s2p_m}(b).$$

The electron transfer probabilities have been calculated within the framework of the continuum distorted wave (CDW) approximation [2]. Calculations for the projectile excitation and ionization probabilities were performed by a semiclassical approximation (SCA)

**X-RAY PHOTOELECTRON AND X-RAY EMISSION STUDIES OF THE ROLE OF THE U 6p,5f-  
ELECTRONS IN CHEMICAL BONDING OF URANYL AND URANIUM FLUORIDES**

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For the first time the high-resolution x-ray O<sub>4,5</sub>(U)- emission spectrum from UO<sub>2</sub>F<sub>2</sub> was measured and its structure was interpreted on the basis of the x-ray photoelectron spectroscopy data and results of theoretical calculations. The fine x-ray photoelectron spectral structure from UF<sub>4</sub> and UO<sub>2</sub>F<sub>2</sub> in the binding energy range 0 - ~50 eV was shown to characterize the outer (OVMO) and the inner (IVMO) valence molecular orbitals due to the interaction of the U 6<sub>p</sub>,5<sub>f</sub>- and L 2<sub>s</sub>,2<sub>p</sub>- electrons of uranium and ligands. This agrees with the results of the theoretical calculations of electronic structure of UO<sub>2</sub>F<sub>2</sub>, was confirmed by the x-ray emission spectroscopy data, and for UF<sub>4</sub> – by the data of the nuclear-electron (conversion) spectroscopy. On the basis of the obtained data the U 5<sub>f</sub> electrons were suggested to participate directly in chemical bonding. The fine x-ray photoelectron spectral structure due to the IVMO electron was shown to characterize the participation degree of electrons from atomic shells in chemical bonding, the structure of the close environment of considered ions, and the bond lengths in compounds. Practically, on the basis of the x-ray O<sub>4,5</sub>(U)- emission spectral data taking into account the x-ray photoelectron fine spectral structure parameters of the low binding energy filled shells of the neighboring uranium and ligand ions, experimental evidence of formation of the inner valence molecular orbitals in uranium fluoride was obtained.

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**THE STUDY OF THE U5f- STATES IN URANIUM OXIDES AND FLUORIDES ON THE BASIS OF THE  
SINCHROTRON RADIATION EXCITED SOFT X-RAY ABSORPTION AND RESONANT EMISSION**

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Near edge x-ray absorption fine structure (NEXAFS) and resonant x-ray emission spectroscopy (RXES) measurements were performed at the U 5d thresholds to study the U 5f states in the uranium metal, fluorides UF<sub>4</sub>, UF<sub>5</sub>, and oxides UO<sub>2</sub>, U<sub>3</sub>O<sub>8</sub>, UO<sub>3</sub>. Direct participation of the U 5f electrons in chemical bonding has been previously observed experimentally by x-ray photoelectron and emission spectroscopies for uranium oxides. In the present work the U 5f states in uranium oxides and fluorides were studied on the basis of the synchrotron radiation excited soft x-ray absorption and resonant emission spectra. On the basis of the obtained data the U 5f electrons were suggested to participate directly in the chemical bonding. The fine emission spectral structure and the ff- excitation effect were shown to be a characteristic of the localization of the U 5f electrons for uranium compounds. Thus, going from UF<sub>4</sub> with the strongly localized 5f electrons to UO<sub>3</sub> with the delocalized 5f electrons, the intensities and number of peaks attributed to ff- excitation decrease. Resonant soft x-ray emission spectroscopy has proven to be an efficient tool in study of the electronic structure of uranium compounds. It provides high resolution reliable spectral data with relatively small amount of uranium samples.

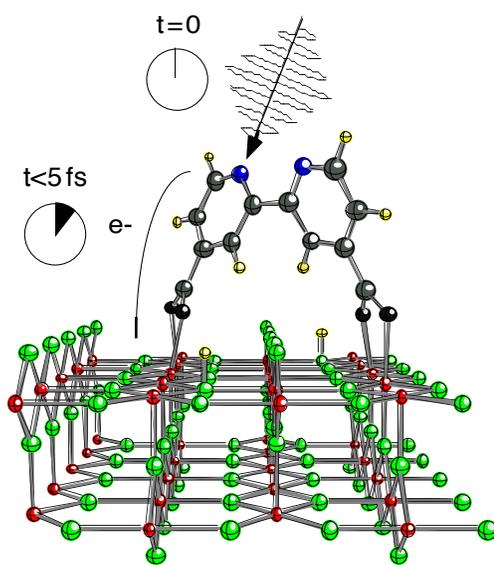
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## Transfer Charge Mapping on Femto-Second Scale

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Core hole decay technique such as autoionisation participator electron spectroscopy provides an internal clock to probe charge transfer in the femto-second scale. Usually performed on weakly interacting adsorbates, this technique has successfully been used on covalent bound systems. N1s autoionisation on Bi-isonicotinic acid/TiO<sub>2</sub>(110) has been recorded to probe charge transfer dynamics from the photoexcited molecular states to the TiO<sub>2</sub>(110) substrate. A careful study of the occupied and unoccupied states allows us to 1) determine the absolute energy separation between the different electronic levels and 2) to investigate the charge transfer from different photoexcited molecular states. Similar systems such as isonicotinic acid, nicotinic acid and picotinic acid on TiO<sub>2</sub>(110) have been studied. The charge transfer from the adsorbate has been investigated depending on the location of the N atom within the molecules.



**'Absorption in Emission' - Radiative Auger effect in silica, phosphate and sulfate**

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Radiative Auger - KLL (RA) spectra from silica, phosphate and sulfate will be presented and compared (as far as possible with real Auger spectra over the same energy range. Much additional structure is seen in the RA spectra which can be interpreted as

- (i) a triplet P K L<sub>2,3</sub> L<sub>2,3</sub> peak which is allowed for RA photon emission but forbidden for Auger electron emission [1], and
- (ii) related to K-absorption spectra, which will also be shown for comparison

The relaxation of a core hole which does not proceed by simple X-ray emission can be thought of as providing the ion with energy which can be used in the following ways:-

- (a) to excite an electron to a bound state and the remaining energy emitted as an X-ray
- (b) used to excite an electron so that it is just ionised but has 'zero' kinetic energy, the remaining energy emitted as an X-ray
- (c) used to excite an electron to the continuum where it will have some kinetic energy, but the remainder emitted as an X-ray.
- (d) wholly used to eject an Auger electron

Processes (a) thru (c) are observed as the 'Radiative Auger Effect'(RAE) with (b) generating an X-ray with the same energy as the Auger electron (d). Processes (a) thru (c) also absorption and so the structure seen in the RAE should correspond to (a) pre-edge absorption fine structure, (b) the 'white line' and (c) NEXAFS. Thus absorption is observed in emission!

Reference

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**New crystals for soft X-ray spectroscopy ( and the curious case of  $n = 0.707$  for octadecyl hydrogen maleate)Title in Upper and Lower Case with Any Credits Denoted with an \***

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The characterization of new crystals with large 2d spacings for soft X-ray spectroscopy will be reported:-

Diocadecyl succinate 2d = 8.9 nm

diocadecyl sebacate 2d = 12.2 nm

and preliminary results showing their application will be given.

Work with a new crystal of octadecyl hydrogen maleate (2d, 6.25 nm) has shown unexpected and weak peaks which can be interpreted as due to anomalous reflections from an 'effective 2d' of  $6.25 \times 1.414$  nm . The intensity is about 0.3% of the normal reflections. However this anomalous reflection can cause serious problems of peak interference at wavelengths shorter than the C K absorption edge

Polarization Dependence of the Soft X-ray Raman Scattering at the L edge of TiO<sub>2</sub>

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Polarization dependence of the soft X-ray Raman scattering is investigated at the Ti 2p absorption edge of TiO<sub>2</sub>. Strong Raman scattering feature appears about 14eV below elastic peaks with strong polarization dependence. These Raman scattering structures are charge transfer excitations to the antibonding state between 3d<sup>1</sup>L<sup>-1</sup> and 3d<sup>0</sup> states, because they are enhanced when the incident photon energies are tuned at satellite structures of Ti 2p absorption edge. Broad Raman scattering structures are found between 3eV and 10eV below elastic peaks. They are assigned to be nonbonding type charge transfer excitations or interband transition from O 2p valence to Ti 3d conduction bands, which includes the crystal field splitting in D<sub>2h</sub> symmetry with two Ti-O bond lengths.

**KLL Auger Transitions in Metallic Cu and Ni \***

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The detailed knowledge of the KLL Auger spectra of Cu and Ni provides important information on the electronic structure of these metals and the accurate determination of the respective high energy Auger parameters is necessary for

estimating charge transfer in their alloys. In the case of overlayer structures using these high energy Auger lines a nondestructive depth profiling of the subsurface and interface regions is possible. From the comparison of high resolution measurements with theory, information can be expected on the nature of the angular momentum coupling, the role of relativistic effects and of initial and final state excitations.

Cu and Ni KLL spectra were excited by Cu X-rays from metallic Cu and Ni layers of 10 nm thickness, vacuum evaporated onto Si wafer substrates [1,2]. High energy electron spectra of in situ Ar ion cleaned sample surfaces were measured by a home built electron spectrometer based on a hemispherical analyzer [3], with an energy resolution of 1.3 eV. High intensity spectra were obtained in addition, using a little worse resolution ( 2.2 eV ), from a serie of thin layer samples, having a layer thickness in the range of 10-60 nm. These spectra proved to be helpful identifying spectral details attributable to intrinsic processes. For energy calibration in the high energy range Cu Ka excited Cu 2p lines were used.

For estimating the systematic error of the correction for the background caused by inelastically scattered electrons, two different kinds of methods were used, the Tougaard-type background correction [4] and the Partial Intensity Analysis model [5]. The evaluated relative transition energies and relative intensities, compared to earlier experimental ( Cu ) and theoretical data , show a reasonably good agreement, however, a significant difference is observed for the respective absolute Auger transition energies [1]. Intensive satellite lines, attributable to initial [6] and final state shakeup processes, have also been identified in the spectra. Although the experimental error of the relative intensities of these satellites is rather high, they seems to be about one order of magnitude more intense than expectable from atomic calculations using the sudden approximation.

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**Electronic Energy Loss Spectroscopy of Individual Nanotubes**

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EELS is a powerful tool for the study of the electronic structure through two investigation channels: absorption edges provide a direct correlation with the unoccupied density of states while the low-loss energy-region contains the signature of individual and collective excitations of the valence electrons. Performing this spectroscopy in the context of a scanning transmission electron microscope (STEM) offers the possibility to obtain a spectroscopic information from a subnanometer volume of the specimen while a dark field image of the analysed object is recorded in parallel. The spectrum image approach [1], developed in Orsay, combines these multi detection abilities with that of scanning the subnanometer probe at the surface of the specimen. Typically, collections of a hundred of individual spectra are acquired by scanning the subnanometer electron probe over nanometer scale areas with an accuracy of 2-3 angstroms in the definition of the location of the probe on the specimen.

Using high spatial resolution EELS, we investigated the local chemistry, the nature of the chemical bonds and the dielectric properties of nanotubes and onions made of various layered materials.

More specifically, this presentation will be divided into three parts:

- 1- Identification of composite nanotubes with a complex structure like coaxial BN-C [2] nanotubes and  $CN_x$  nanotubes using the spectrum image mode.
- 2- Determination of the nature of the chemical bond in single shell nanotubes and  $CN_x$  nanotubes. This involves a discussion on the effects on the electronic structure of the graphene sheet curvature [3] and of the introduction of nitrogen atoms in the carbon hexagonal network.
- 3- Study of valence electron excitations in carbon,  $MoS_2$  and  $WS_2$  multishell nanostructures of cylindrical or spherical geometry (nanotubes and onions). We will focus mainly on a study of the probability of excitation of surface modes as a function of the coupling distance between the subnanometer probe and surface of the nano-objects [4]. Some results on single-shell carbon nanotubes and ropes of single-shell carbon nanotubes will be also discussed.

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**Photoelectron Spectroscopy at Ten Torr**

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We report on the development of a new photoelectron spectrometer capable of operating at pressures up to at least 10 Torr. In this instrument a sample is placed in front of a small aperture at the apex of a conical lens or "nozzle" and illuminated by a photon beam that enters the sample cell through a silicon nitride window. Photoelectrons emitted from the sample pass through the aperture, along with a supersonic jet of gas molecules from the sample cell. The aperture is the opening of a differentially pumped electrostatic transfer lens. This lens transports electrons from the sample surface to the source plane of a commercial hemispherical energy analyzer while passing through two stages of differential pumping. The gas pressure at the energy analyzer is more than seven orders of magnitude lower than in the sample cell, so the analyzer remains in high vacuum. Although the photoelectrons are attenuated through scattering by gas molecules in the sample cell and in the supersonic jet, quite reasonable count rates can be obtained in a wide range of experimental conditions.

The design and performance of our new instrument will be discussed, and the results of some preliminary experiments will be presented using several different photoemission techniques, including core and valence level spectroscopy and Auger-yield NEXAFS measurements.

**High-temperature order-disorder phase transitions on the Si(100) surface monitored by  
high-temperature photoemission spectroscopy**

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High-temperature phase-transitions have been observed on the surfaces of the elemental semiconductors Ge(111), Ge(100), Ge(110), Si(110), Si(111), and Si(100) [1]. On this last surface, the room temperature (2X1) reconstruction is characterized by the presence of Si-Si dimers resulting from the bonding of two topmost-layer silicon atoms. The behavior of the dimerized surface at higher temperatures has been investigated in the past by various techniques. HREELS and He I valence-band PES experiments [2] showed the onset of surface metallization for  $T > 900\text{K}$ . Reflection electron microscopy [3] studies suggested the presence of a roughening transition at 1455K. He diffraction experiments [1] showed evidence of structural change on the surface at about 930K. Photoelectron diffraction data [4] revealed the presence of a phase transition at about 1400K, which was interpreted as being due to incomplete surface melting. Surface melting takes place when the thickness of the disordered layer does not monotonously increase as  $T$  is approaching the bulk melting temperature  $T_m$ .

In this work we present a synchrotron radiation valence band photoemission spectroscopy study of the Si(100) surface from room temperature up to about 1660K, i.e. close to  $T_m$  (1685K). The experiments were carried out using synchrotron radiation on the undulator TGM5 beamline at the BESSY I storage ring in Berlin. The results show considerable emission intensity at the Fermi edge as the temperature is increased, indicating strong metallic character of the surface at high temperatures. The metallicity of the surface is attributed to dimer dynamics effects induced by the flipping and twisting motion of the dimers, to electron-phonon interaction and, at higher temperatures to the partial breaking/rebonding of the dimers [4]. The data also indicate a phase transition taking place at about 70K below the bulk melting point. It is possible that either further dimer building blocks break down or, similarly to the Ge(111) [1], the Si(100) surface undergoes incomplete surface melting above 1610K.

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**A magnetic dichroism study of Fe nanostructures on c(2x2)N/Cu(100) surface**

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It is known from scanning tunnelling microscopy experiments that at saturation coverage adsorbed N atoms on Cu(100) form square islands of c(2x2) periodicity and about 5nm x 5nm in size [1]. These islands can self organise in regular patterns. Deposition of Fe on this surface leads to formation of Fe islands in areas not passivated by N atoms. The Fe islands form regular structures upto 10 atomic layers deep [2].

In the present study, we have examined the magnetic properties of the surface by means of Fe3p magnetic linear dichroism in angular distribution (MLDAD) and magnetic circular dichroism (MCD). The results show a magnetic dependence on island size and distribution.

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**Reactive Plasma Spray For The Deposition Of Ti/Tin Coatings: A Comparative Compositional Study By X-Ray Diffraction And X-Ray Photoelectron Spectroscopy.**

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This paper reports the result of a study aimed at determining the composition of Ti/TiN coatings deposited by reactive plasma spray (RPS). The coatings were obtained by spraying titanium powder in a low pressure N<sub>2</sub>/Ar atmosphere. The resulting film has a variable nitrogen content in the form of titanium nitrides, depending on experimental parameters such as the gas partial pressure, total pressure, distance sample-source, etc. The determination of the composition of the film can be obtained in principle by various methods. Here we have performed a comparative compositional study using X-ray photoelectron spectroscopy and X-ray diffraction. We found that the two techniques provide very similar results and hence either one can be used for the compositional characterization of these coatings.

**Structural studies by X-Ray Photoelectron Diffraction of electrochemically grown CdS films on Ag(111) and Ag(100) substrates.**

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The structure and chemical composition of electrodeposited CdS films on Ag(111) and Ag(100) substrates has been studied by X-ray photoelectron spectroscopy (XPS), and X-ray photoelectron diffraction (XPD). The CdS films were prepared by the electrochemical atomic layer epitaxy (ECALE) method, alternating underpotential deposition (UPD) cycles of sulphur and cadmium from solution precursors. The XPS spectra of the sulphur 2p line indicated that only the S  $^{2-}$  component is present on the CdS films, no evidence for oxidation in air was observed. XPD measurements were performed by measuring the angle dependence of the S 2p, Cd 3d  $_{5/2}$  and the Ag 3d  $_{5/2}$  peak intensity. The comparison of the experimental XPD patterns with single scattering-cluster (SSC) calculations showed that the CdS film has a wurzite-type structure (hcp), both on Ag(111) and Ag(100), with the basal (0001) plane parallel to the substrate surface. For this wurzite layer, two bulk truncated terminations are possible: one containing only S atoms and the other only Cd atoms. The XPD results indicate that the CdS film has a Cd layer termination. The XPD patterns measured for the CdS film deposited on Ag(111) show a 6-fold rotational symmetry, whereas those for Ag(100) show a 12-fold rotational symmetry. The latter result can be explained with the growth of equivalent domains of CdS oriented with the (0001) plane parallel to the Ag(100) surface. The CdS films grows on the Ag(100) plane with the CdS[10-10] direction parallel to the Ag [010] direction.

**Formation Of Linear Metal-Plasma X-Ray Source For Producing Low-Photon-Energy Quasi-X-Ray Lasers Using A Capillary**

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The low-photon-energy flash x-rays such as the water-window x-rays are useful in order to perform x-ray microscopy of organisms, and several condenser-discharge generators have been designed. In order to increase the intensity of low-photon-energy characteristic x-rays, the effective electron accelerating voltage should be decreased as low as possible even when a higher condenser charging voltage is selected. In view of this situation, the surface-discharge capillary is quite useful to decrease the voltage and to generate stable discharges, and the linear plasma x-ray source can be formed. Using this capillary, the characteristic x-ray intensity may increase with corresponding increases in the capillary length by the conversion of bremsstrahlung x-rays into fluorescent rays. In our research, we have formed the linear metal-plasma x-ray source for producing low-photon-energy characteristic x-rays such as quasi-x-ray lasers.

This flash x-ray generator is composed of a high-voltage power supply, a polarity-inversion ignitron pulse generator, an oil-diffusion pump, and a radiation tube with a capillary. The high-voltage condenser of about 200 nF in the pulse generator is charged up to 20 kV by the power supply, and the electric charges in the condenser are discharged to the capillary in the tube after closing the ignitron. In the present work, the pump evacuates air from the tube with a pressure of about 1 mPa. Both the cathode voltage and the discharge current displayed damped oscillations, and x-rays were produced during the damped oscillations. The first peak current had a value of about 4 kA, and the effective x-ray duration was less than 0.02 ms.

**High-Photon-Energy Quasi-X-Ray-Laser Production From Plasma X-Ray Source**

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With recent advances in the high-voltage pulse technology, the soft x-ray lasers have been produced using the discharge capillary. However, it is quite difficult to produce the x-ray lasers in the higher-photon-energy region of about 10 keV or over. In the cases where the flash x-ray generators are employed, although high-intensity bremsstrahlung x-rays are produced corresponding to the time dependence of the tube voltage and current in the flash x-ray tube, the bremsstrahlung x-rays can be absorbed by the plasma x-ray source which consists of metal ions and electrons. In view of this situation, the characteristic x-ray enhancement may be performed when the bremsstrahlung rays are effectively absorbed and are converted into fluorescent x-rays. For this research, we have designed a plasma flash x-ray generator in order to produce high-intensity quasi-monochromatic x-rays such as quasi-x-ray lasers.

The plasma flash x-ray generator employs a high-voltage power supply, a low-impedance coaxial transmission line, a high-voltage condenser with a capacity of 200 nF, a turbo-molecular pump, a thyristor pulser as a trigger device, and a flash x-ray tube. The high-voltage main condenser is charged up to 60 kV by the power supply, and the electric charges in the condenser are discharged to the tube after triggering the cathode electrode. The flash x-rays are then produced. As the electron flows from the cathode electrode are roughly converged to the target by the electric field in the tube, the plasma x-ray source which consists of metal ions and electrons forms due to the target evaporating. In the present work, the peak tube voltage was almost equivalent to the initial charging voltage of the main condenser, and the peak current was less than 30 kA. The characteristic x-ray intensity substantially increased according to the growth in the plasma x-ray source. When the plasma x-ray source grew, the bremsstrahlung x-rays were absorbed and were converted into fluorescent rays, and high-intensity characteristic x-rays were produced.

Xps And Xes Investigations Of D-P Resonance In Some Copper Halcogenides

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The investigation of  $A_{2-x}B^VI$  copper tellurides and selenides electron energy spectra seem to be very interesting because of considerable sensitivity of the  $A_{2-x}B^VI$  electrophysical and optical properties to the stoichiometry of this deficient alloys.

The cation sub-lattice disorder in  $A_{2-x}B^VI$  causes the formation of homogeneous areas on the state diagram whenever a deviation from stoichiometry takes place. The conductivity type is defined by the excess atoms of copper, tellurium orelenium behaviour. Copper vacancy formation and their further ionisation always bring about the p-type conductivity.

Ab initio theoretical calculations for these non-stoichiometric  $A_{2-x}B^VI$  compounds are difficult due to the existence of 3d-electrons in copper. That is why the investigation of their band structure and electron density by means of XPS and XES proves to be of principal importance.

Earlier we pointed out that the resonance interaction between copper d-states and non-metal p-states (d-p resonance) in binary and ternary compounds leads to splitting of non-metal p-states into two components and repulsing the latter apart from the copper d-band. The magnitude of this p-band splitting increases almost linearly with increase of the amount of copper in the compounds. At the same time the narrowing of the band gap is elucidated by the rise of the top of valence band which is formed by one of the split p-subbands with the admixture of copper d-states. Still XPS spectra were obtained for few samples of Cu-Se and Cu-Te systems.

At the present moment the spectra of binary  $Cu_2Se$ ,  $Cu_{1.84}Se$ ,  $Cu_{1.82}Se$ ,  $Cu_2Te$ ,  $Cu_{1.95}Te$ ,  $Cu_{1.9}Te$ ,  $Cu_{1.7}Te$  and ternary  $CuInSe_2$  are obtained and matched in a common binding energy scale with XES (matched by the core state of tellurium 4d 5/2 or selenium 3d; the matching accuracy being  $\sim 0.5eV$ ).

The results of this matching show that with the increase of the amount of copper in the binary compounds studied there appears the increase of the distance between the components of the split p-band. Copper 3d-states appear in the centre of the tellurium or selenium p-band, split it into two components nearly symmetrical about the d-band which

contributes into each of the components ('structure' in the XPS). The increase of the amount of copper results in a slight re-distribution of intensity of the components of p-band, growth of the magnitude of p-band splitting which is mostly due to the repulsion of the upper p-subband by the d-states and the narrowing of the band gap. All the results completely fit the d-p resonance model.

**Medium Energy Range HREELS as a tool for analytical and structural determination of solid surfaces**

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REELS were used in the medium energy range (1-5 keV) to study the possibility of determination of materials composition in some special cases of solids (amorphous, polycrystalline, single crystal).

The new experimental method to get important material parameters for the surface analytical methods (AES, XPS, REELS) and for the structure determination of single crystals by AED, XPD, AEH, XPH is discussed phenomenologically, assuming the independent oscillator model of the solid in harmonic approximation.

The sensitivity and the limits of the method are also discussed through special examples. Spectra of elements and some compounds, which are important technological applications point of view, are presented as examples.

The physical parameters, which can be deduced with the new surface science method, are crucial not only in the quantitative analysis but in the diffraction and holographic methods as well giving new perspectives for the nondestructive HREELS surface science method in the future studies of nanometer scale material structures.

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The effect of annealing time on the electronic and atomic structures of the Fe-Cu-Nb-Si-B alloys

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Three nanocrystalline (*nc*-)  $\text{Fe}_{73.5}\text{Cu}_{1}\text{Nb}_{3}\text{Si}_{13.5}\text{B}_{9}$  alloy samples (denoted by FCNSB30, FCNSB60, and FCNSB120) were obtained from the amorphous (*a*-)  $\text{Fe}_{73.5}\text{Cu}_{1}\text{Nb}_{3}\text{Si}_{13.5}\text{B}_{9}$  by an annealing temperature of 550C for 30, 60, and 120 min, respectively. X-ray absorption near-edge-structure (XANES) and extended x-ray absorption fine structure (EXAFS) spectra of these alloys were measured at the Fe  $L_{3,2}$  and  $K$ -edges using the sample drain current mode and the transmission mode at room temperature. The intensity in the Fe  $L_{3,2}$ -edge XANES spectrum of *nc*-FCNSB changed significantly with the increase of the annealing time indicating that the annealing time strongly influences the Fe  $3d$  local electronic structure. Closely examining the Fourier transformation of the Fe  $K$ -edge EXAFS spectra of *nc*-FCNSB reveals that the stable crystalline structure of the Fe-Cu-Nb-Si-B alloys can be obtained by an annealing time of 60 min. The enhanced crystallization of the Fe-Cu-Nb-Si-B alloys under the optimum annealing condition improves the magnetic properties of the *nc*-FCNSB alloys.

**Photoemission Studies of Self-Energy Effects in Strongly Correlated Materials**

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Recent instrumentation developments in photoemission are providing new insights into the physics of complex materials. With increased energy and momentum resolution, it has become possible to examine in detail different contributions to the self-energy or inverse lifetime of the photohole created in the photoexcitation process. This information may be extracted either from momentum distribution curves, the photoemitted intensity as a function of momentum at constant binding energy, or from the more traditional energy distribution curves, the intensity as a function of binding energy at constant angle or momentum. In studies of metallic systems, including Mo and 2H-TaSe<sub>2</sub>, it is possible to isolate and identify the different contributions to the quasi-particle lifetime including electron-electron, electron-phonon and electron-impurity scattering. In contrast to these systems, studies of the high T<sub>c</sub> superconductor, Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8</sub>±?, show that the material behaves like a non-Fermi liquid rather a Fermi liquid. Further detailed studies of the latter material reveal that interactions with magnetic excitations in the system lead to strong renormalization effects at the superconducting transition.

This work has been carried out in different collaborations with Tonica Valla, Alexei Fedorov, Barry Wells, Zikri Yusof, Jinue Xue, Kevin Smith, Qiang Li, Genda Gu, N. Koshizuka, and Frank DiSalvo. The work at BNL is supported by the Department of Energy under contract number DE-AC02-98CH10886

**Penning Ionization of Amides by Collision with He\*(2<sup>3</sup>S) Metastable Atoms**

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Japan

Abstract:

Penning ionization of amides (formamide, acetamide, and thioacetamide) upon collision with He\*(2<sup>3</sup>S) metastable atoms was studied by collision-energy-resolved Penning ionization electron spectroscopy. Partial ionization cross sections were found to be larger for ionization from molecular orbitals having electron density around the C=O and C=S groups. Collision energy dependence of partial ionization cross sections indicates that interaction potentials are highly anisotropic between He\*(2<sup>3</sup>S) atoms and amides investigated in this study. The larger negative collision energy dependence of  $\sigma$  C=O bands than  $\pi$  band shows that attractive interactions are larger around the oxygen atom for the in-plane direction rather than the out-of-plane direction. On the contrary, the larger negative collision energy dependence for ionization from sulfur 3p orbitals than the sigma C=S band indicates that an attractive interaction around the sulfur atom was larger for in-plane or out-of-plane directions vertical to the C=S axis. Weak interactions around the nitrogen atoms were similar to the conjugated systems of urea and thiourea in a previous study, which is different from the strong attractive interaction around the 'lone pair' orbital region of amine. Repulsive interactions were found around the methyl group of acetamides, which results in small partial ionization cross sections and smaller negative collision energy dependence of  $\sigma_{\text{CH}}$  bands.

**Cross sections for elastic scattering and bremsstrahlung of fast electrons scattered by C<sub>60</sub>\***

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The differential cross sections (DCS's) for the scattering of fast electrons by C<sub>60</sub> have been calculated. To describe this process, the real fullerene potential formed by the superposition of the atomic fields is replaced by a phenomenological potential V(r). V(r) is assumed to be nonzero within an infinitely thin spherical layer with radius equal to that of the fullerene [1,2].

The effective depth of this potential well is chosen so as to yield an electron affinity equal to the experimental value, I= 2.65 eV [3]. Within the framework of this model two experimental parameters R=6.639 a<sub>0</sub> and I fully define the spectrum of the electronic states in this potential well.

The general expression for the electron scattering amplitude and the differential cross sections were derived within the first Born approximation (FBA). In this approach they are described by simple analytical formulae. According to the FBA the DCS at zero scattering angle is independent of the electron energy and equal to a constant proportional to the jump of the logarithmic derivative of the wave functions at the boundary of the potential well. The numerical calculations were performed for the DCS as a function of scattering angle at different values of electron impact energies.

The expressions for the DCS were used to derive formulae for the diffusion and the bremsstrahlung (BS) cross sections for the electron scattered by the potential V(r). For photon energies much smaller than the electron kinetic energy these cross sections are connected to each other by the so-called low energy theorem [4]. The numerical calculations show the oscillatory behavior of the BS cross section as a function of electron energy. This unexpected result is due to the features of the atomic structure of the carbon cluster and deserves to be studied experimentally.

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Elastic electron scattering by  $C_{60}$  at low energy\*

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Within the framework of a Dirac bubble potential model of the fullerene [1,2] the total and differential cross-sections (DCSs) of slow electrons scattered by  $C_{60}$  have been calculated. According to this model, two experimental parameters, namely the fullerene radius  $R=6.639 a_0$  and the electron affinity energy  $I=2.65$  eV, define the spectrum of the electronic states of  $C_{60}$ . It was shown that in this potential well there are two excited p- and d- bound states with energies 1.94 eV and 0.68 eV, respectively, and that the continuum is described by some linear combination of the spherical Bessel functions [2]. The coefficients of this combination are determined by matching conditions of the continuum wave functions inside and outside of the potential sphere. The expression for the phase shifts was derived and involves the jump of the logarithmic derivative of the wave functions  $dL$ . It was shown that the magnitude of  $dL$  at the boundary of the potential well is connected with the fullerene parameters  $R$  and  $I$  [2].

The cross sections of slow electrons scattered by  $C_{60}$  are defined by the first few phases. Our calculation shows that for electron energies from 0 to 14 eV it is sufficient to take into account only the first six phases. We found that the total cross section of  $C_{60}$  for zero energy is one and a half times larger than the geometric cross section. The existence of excited bound states leads to the appearance of resonances connected with the quasi-discrete levels formed by a centrifugal potential barrier. Similar resonances were found in measurement [4], where they were attributed to shape resonances.

The DCSs were calculated as a function of the both scattering angle for fixed electron energy, and as a function of energy for some values of the angle. Comparison of these cross sections with available experimental data [5] and results of molecular calculation [6] indicates qualitative agreement.

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Two-Dimensional Penning Ionization Electron Spectroscopy of CO/He\*(2<sup>3</sup>S)

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From a two-dimensional Penning ionization electron spectrum (2D-PIES), some details about stereo reaction dynamics of atom-molecule collisional reactions involving excitation energy transfer and electron transfer can be studied. In this study, 2D-PIES of CO/He\*2<sup>3</sup>S were measured by using the apparatus reported previously [1]. Classical trajectory calculations were performed in order to obtain calculated 2DPIES, and the calculated 2D-PIES was compared with the observed result. Interaction potential energy surfaces were calculated for the entrance channel with the CCSD(T) method and exit channel with the MRCI and the OVGf methods. Anisotropic entrance potential surface obtained by using a Li atom instead of He\* was adapted to reproduce collision energy dependence of partial ionization cross sections by two-dimensional Penning ionization electron spectroscopy. Based on the electron exchange mechanism [2], electron transition probabilities of the positional dependence were proportional to the square of overlap integrals between He 1s orbital and ionized molecular orbitals. Their proportional constants were decided for three ionized molecular orbitals in order to reproduce observed ionization branching ratios. The absolute values of the potential energies for exit channels were corrected by measured ionization potentials. By adding up the electron transition probabilities for the specific electron energy calculated by the difference between potential energies for the entrance and the exit channels at each trajectory step, the collision-energy-resolved Penning ionization electron spectrum (CERPIES) was obtained. The CERPIESs calculated at various collision energies were then converted into a theoretical 2D-PIES.

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**Non-dipole and elastic scattering effects in X-Ray photoemission\*)**

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The published experimental and theoretical results on non-dipole parameters for photoelectron angular distribution are reviewed and discussed. Based on the Dirac-Fock-Slater calculations for non-dipolar parameters of all electron subshells in elements from H up to Xe. the regular and specific behavior of this parameters for ns-, np- and nd- subshells is considered and found regularity explained using analytical expressions for parameters. The specific behavior is observed near Cooper minimum and in some other cases. The experimental determined non-dipolar parameters agree with calculations. In some cases the high order perturbation theory must be applied to get good correspondence with experiment.

Using transport theory approach for the account of elastic scattering the contribution of non-dipolar transitions to photoelectron angular distribution in solids is derived and comparison with Monte-Carlo simulations is presented for polarized and unpolarized excitation sources. The modification of angular distribution going from gas to solids is similar to that observed for dipolar transitions.

The non-dipolar transitions make considerable contribution to the intensity especially near magic emission angle and should be taken into account while performing XPS quantitative analysis or X-Ray standing wave method. If these contributions are ignored the error in XPS- analysis can amount up to 15%. Considerable errors are also expected in X-Ray standing wave method because the X-Ray photoelectron intensity depends on the mutual direction of photoelectron and X-Ray flux due to non-dipolar transitions. The forward/backward asymmetry factors

determined in X-Ray standing wave experiments are in a good agreement with Dirac-Fock-Slater calculation

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**Comparative Investigations Of Structure And Photoluminescence Of Si Low-Dimensional Systems**

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Creation of the silicon nanocrystal systems attracts great attention now due to the perspective of the development Si based optoelectronic devices. Silicon nanocrystal structures, like porous silicon (PSi) and Si nanoparticles in silicon oxide films, prepared by different technological regimes, have been studied.

X-ray photoelectronic spectroscopy (XPS), Atomic Force Microscope (AFM), photoluminescence (PL) and photoluminescence excitation (PLE) methods, as well as electron paramagnetic resonance (EPR) have been used for investigation the mechanism of the photoluminescence and it's excitation in such systems.

We have shown that PSi red PL band could be decomposed on two elementary bands: ( $h\nu_{m1}=2.1\text{eV}$ ,  $h\nu_{m2}=1.9\text{eV}$ ). The UV light mainly excites the former one with wavelengths  $\lambda$  from 250-350nm spectral ranges. The visible light from the 350-550 nm range excited the second one predominantly.

We have observed by XPS that the decrease of anodization current density up to 10 mA/cm<sup>2</sup> leads to the increase of the silicon sub oxide content on the PSi surface mainly nearly Si/SiO<sub>x</sub> interface. At the same time, as follow from AFM results, the PSi has essential roughness and lowest diameter of the Si wires nearly 20nm. These PSi samples are characterized by the intensive red PL with  $h\nu_{m2} = 1.9\text{ eV}$  and also highest density of the dangling bonds (DB), equal 4-5  $10^{13}\text{ cm}^{-2}$ . The late fact is the evidence of highest surface area.

It has been found the increase of the anodization current density leads to the PSi roughness decrease and the polishing of the PSi surface layer. Simultaneously, the intensity of the red PL band decrease and the first band with  $h\nu_{m1}=2.1\text{eV}$  start dominate. These samples are characterized by low density of dangling bonds, equal 1-2  $10^{13}\text{ cm}^{-2}$ , and also the mainly silicon dioxide contents on the PSi wire surface.

The mechanisms of the both luminescence bands in PSi have been discussed and analyses. The comparative investigation of the PL peculiarities for Si nanoparticles in silicon oxide films has been used for confirmation of the proposed luminescence models.

The electronic structure of  $K_6C_{60}$  studied by soft x-ray spectroscopy

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The electronic structure of  $C_{60}$  and potassium doped  $C_{60}$  films have been studied by soft x-ray absorption and emission spectroscopies. There are significant changes in the XAS spectrum upon doping of potassium. The C  $1s$  absorption spectrum of potassium doped  $C_{60}$  shows less prominent  $\pi$  absorption resonances as compared to  $C_{60}$ . The trend is in agreement with other XAS measurements. The intensity contributed from the LUMO is reduced since the LUMO becomes occupied upon potassium doping, while the resonances of the K  $2p \rightarrow 3d$  absorption (at about 297.4 eV) increases. The C  $K\alpha$  emission spectrum of doped  $C_{60}$  shows a resolved filled LUMO ( $t_{1u}$ ) derived valence band. The intensity ratio of HOMO-derived band to LUMO-derived band is 2, indicating that a  $K_6C_{60}$  phase is forming the potassium doped  $C_{60}$  film. Small variations with excitation energy in the spectral shape compared to solid  $C_{60}$  suggests that resonant inelastic x-ray scattering becomes less prominent due to the formation of metallic system upon potassium doping. Nevertheless, the remaining of some shape variations in the photon-excited emission of  $K_6C_{60}$  suggests the existing of a certain degree of molecular character.

**Relaxation Of Core Excited Molecules Probed By Auger Ion Coincidences**

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The development of photon beamlines and high luminosity electron analyzers 1 has opened new opportunities for high resolution Auger electron-ion coincidences spectroscopy.

The Auger-ion coincidence technique has been shown to be an unique tool for probing fragmentation 2. Indeed, in this kind of study, it is essential to disentangle between the states of different energies, before the ion undergoes dissociation. Conditions for observing selective fragmentation will be discussed.

In the case of resonant excitation, photon energy selection allows to promote a core electron not only into a specific empty orbital, but also to excite particular vibrational modes. We will review studies showing that nuclear motion can play a significant role within the lifetime of the core excited states in the case of polyatomic molecules 3,5. Dissociation can be indirectly mediated through geometry changes. As a result, fragmentation of an ion depends not only on its internal energy, but also on the way it has been produced.

Angular distribution properties of the emitted particles are also relevant to obtain a full dynamical description of the core relaxation process. We have developed a set up devoted to angle-resolved Auger electron spectroscopy from fixed-in-space molecules 6. The photon energy dependance proves that photoionization and Auger decay have to be coherently treated 7.

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**Biomedical surfaces studied by x-ray photoelectron spectroscopy in combination with static secondary ion mass spectrometry**

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X-ray photoelectron spectroscopy (XPS) has been applied for over 30 years to study biomedical problems. Certainly, its quantitative, information-rich nature has assisted in solving numerous problems. However, as the biological sciences continue to assume increasing importance in most areas of technology (materials, medicine, computation, catalysis, etc.), the limitations of XPS become clearer. To solve modern biology and biomedical problems, we need tools to probe the rich information coded within proteins, polynucleotides, sugars, etc. In addition to composition, we need information on sequence, conformation, orientation, ordering and micron and nanometer spatial arrangement. Secondary ion mass spectrometry (SIMS) in the static mode can be used in complement with XPS to deliver precise details about many systems of scientific and technological importance. Furthermore, ideal analytical tools will deliver this information from a hydrated (biologically relevant) surface. This lecture will present examples of the use of contemporary XPS and SIMS instruments to approach the surface study of supramolecular self-assembled systems, proteins at interfaces, biomaterials and biologically derived materials. The talk will also highlight the use of powerful multivariate statistical tools to extract information from the complex data sets acquired from biological systems.